1,3-Propanediol, diacetate 628-66-0 | DTXSID30211889

Model Performance

Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 8.64e-01

Global applicability domain: Inside

Local applicability domain index: 7.32e-01

Confidence level: 8.39e-01

Nearest Neighbors from the Training Set

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Diethyl propanedioate Measured: 0.96 Predicted: 8.73e-01

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Dimethyl glutarate Measured: 0.62 Predicted: 7.46e-01

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Diethyl butanedioate Measured: 1.20 Predicted: 1.04

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Dimethyl adipate Measured: 1.03 Predicted: 1.03

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Dimethyl succinate
Measured: 0.35
Predicted: 3.94e-01